

CHLORANTHALACTONE A
66395-02-6 | DTXSID90318686

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 43.7 °C

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 3.74e-01

Nearest Neighbors from the Training Set

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2,3:4,5-Bis(2-butylene)tetrahydro-2-furaldehyde
Measured: -80.0
Predicted: -28.4

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2,3-Dimethyl-1,4-naphthoquinone
Measured: 127
Predicted: 108

Image not found

Dibenzosuberone
Measured: 30.0
Predicted: 68.7